Monte Carlo Ray Tracing of Scanning Coherent Diffractive Imaging

Fevola, G.; Ramos, T.; Knudsen, E. B.; Carbone, G.; Andreasen, J. W.

Publication date: 2019

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.
MONTE CARLO RAY TRACING OF SCANNING COHERENT DIFFRACTION IMAGING

G. Fevola¹, T. Ramos¹, E. B. Knudsen², G. Carbone³, and J. W. Andreasen*¹
¹ Technical University of Denmark, DTU Energy
² Technical University of Denmark, DTU Physics
³ MAX IV Laboratory
*e-mail: jewa@dtu.dk

INTRODUCTION: Coherent diffractive imaging (CDI) techniques have gained significant momentum in recent years, and most synchrotrons have dedicated beamlines for CDI techniques, with full-field CDI and ptychography among the most commonly applied. Simulations of CDI experiments can assist in interpretation of data by helping to distinguish signal from noise, or allow design of experiments that minimize X-ray dose. Several factors are however hampering simulations in a ray tracing framework, and so far only simplified test-cases have been reported.

EXPERIMENTAL: We implemented strategies for correct and efficient simulation of diffraction, i.e. enacting Huygens principle by a Monte Carlo process that maximizes yield of computational effort. The sample is specified in terms of its transfer function as a 2D mask of refractive indices. Some meaningful test cases are considered, and the validity of the diffraction patterns then obtained is examined by comparison to expected theoretical expressions, or by inspection of the reconstructions.

RESULTS AND DISCUSSION: We show that diffraction patterns of gratings are properly computed and closely follow the expected theoretical trends; the full-field CDI patterns can be Fourier transformed yielding a noisy version of the initial object; the ptychographical data-set produced by McXtrace (Figure) can be effectively reconstructed by a standard phase retrieval algorithm (ePIE¹, difference map²).

CONCLUSIONS: We detail and discuss the new CDI simulation capabilities of McXtrace³, with a particular focus on ptychography. Ongoing work aims at assessing the signal to noise ratio (SNR) of simulated diffraction patterns of a volume of refractive indices, representing realistic volumetric samples.

REFERENCES:

ACKNOWLEDGEMENTS: J. W. Andreasen and G. Fevola acknowledge the European Research Council for financial support.

Transmission images (top) and diffraction patterns (bottom) from the ptychographical dataset of a simulated concentrical raster scan (right).